

Abstract Submitted
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Pressure-induced rheological transition of polymer melt LUCA DI MARE, JANET WONG, Imperial College London — Experiments have recently shown that a critical normal stress exists where the flow of a polymer melt under shear transits from Couette flow to plug flow as the normal stress exerted onto the melt increases. It has been conjectured that the observation is related to pressure-induced glass transition of the polymer melt. Experimentally this is challenging to verify. Hence MD simulations are carried out to elucidate the origin of such transition. The simulation consists of model polymer chains being sheared between two hard walls under isothermal conditions. The conformation, the density distribution, the dynamics of the chains, the viscosity of the melts, and the through-thickness velocity profiles are simulated by varying the shear velocity, the molecular weight of the chains and its distribution, and the normal stress of the system. The simulated results are then compared with experimental observations. Preliminary results show that the through-thickness viscosity of the melt is heterogeneous under high normal stress conditions. This can result in non-linear velocity profiles resemble experimental findings.

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